

APPLICATION OF PRINCIPAL COMPONENT ANALYSIS TO NIR SPECTRA OF PHYLLOSILICATES: A TECHNIQUE FOR IDENTIFYING PHYLLOSILICATES ON MARS. E. B. Rampe¹ and N. L. Lanza², ¹NASA Johnson Space Center (2101 Nasa Parkway, Houston, TX 77058, elizabeth.b.rampe@nasa.gov), ²Los Alamos National Laboratory (30 Bikini Atoll Rd Los Alamos, NM 87545, nlanza@lanl.gov).

Introduction: Orbital near-infrared (NIR) reflectance spectra of the martian surface from the OMEGA and CRISM instruments have identified a variety of phyllosilicates in Noachian terrains [1,2]. The types of phyllosilicates present on Mars have important implications for the aqueous environments in which they formed, and, thus, for recognizing locales that may have been habitable. Current identifications of phyllosilicates from martian NIR data are based on the positions of spectral absorptions relative to laboratory data of well-characterized samples and from spectral ratios [3]; however, some phyllosilicates can be difficult to distinguish from one another with these methods (i.e. illite vs. muscovite [4]). Here we employ a multivariate statistical technique, principal component analysis (PCA), to differentiate between spectrally similar phyllosilicate minerals. PCA is commonly used in a variety of industries (pharmaceutical, agricultural, viticultural) to discriminate between samples [5]. Previous work using PCA to analyze raw NIR reflectance data from mineral mixtures has shown that this is a viable technique for identifying mineral types, abundances, and particle sizes [6]. Here, we evaluate PCA of second-derivative NIR reflectance data as a method for classifying phyllosilicates and test whether this method can be used to identify phyllosilicates on Mars.

Methods: PCA identifies the spectral variations generated from each sample and reduces the number of dimensions in the data in order to identify the spectral features of greatest importance. Data are reprojected along the axes of greatest variation, called principal components (PC). A score is calculated along each principal component axis for each sample that is a linear combination of feature intensities weighted by relative importance in the model. Because the score is related to spectral features, materials with similar compositions will plot close to one another in PCA scores space. With the correct training set, PCA can predict the mineralogic composition of the sample by anchoring the model to samples with known compositions. Here, the training set consists of USGS geologic NIR reference spectra [7]. Models were made using the commercially available Unscrambler statistical software. We analyzed NIR spectra from 2-2.5 microns because it is in this wavelength region where diagnostic metal-OH absorptions occur. By analyzing second derivatives in this spectral range, effects of continua

are reduced and overlapping absorptions can be resolved [8].

Datasets: We created individual PCA models of three different sets of data: USGS standards, laboratory data of physical mixtures, and currently available martian remote sensing data. The first model of NIR spectra of phyllosilicates from the USGS library [7] was performed to determine the ability of PCA to separate phyllosilicates, particularly ones with similar spectra (e.g. illite and muscovite, smectites of different compositions, and kaolin minerals). We also analyzed NIR spectra of physical mixtures of illite and montmorillonite to examine the ability of PCA to identify variations in phyllosilicate abundances. Finally, we performed PCA on CRISM NIR data from Nili Fossae showing evidence for illite or muscovite [2,4], using USGS illites and muscovites as the training set, to determine if PCA can elucidate the phyllosilicate composition in this region.

Results:

PCA of USGS Clays. The first PCA model can distinguish between NIR data of different phyllosilicates. A scores plot shows that spectrally similar phyllosilicates (e.g. illite vs. muscovite, saponite vs. nontronite, and kaolin minerals) are statistically separable (Fig. 1).

PCA of phyllosilicate mixtures. The second PCA model of NIR data from physical mixtures of illite and montmorillonite correctly clustered the samples by the relative proportions of illite-to-montmorillonite (Fig. 2), with the Al-OH absorption feature having the greatest influence over the sample location in PC space.

PCA of terrestrial and martian illite and muscovite. The third PCA model of NIR data from terrestrial illite and muscovite and from illite/muscovite-rich regions in Nili Fossae show that the martian data plot close to terrestrial illite data, rather than the muscovite data (Fig. 3). This suggests that this region of Nili Fossae may contain illite rather than muscovite, indicating that past aqueous processes were pedogenic rather than magmatic or metamorphic.

Discussion: The three PCA models presented here demonstrate that PCA can correctly differentiate between a variety of different types of phyllosilicates. Despite their spectral similarity, illite and muscovite are well separated in PC space (Fig. 3). When illite and montmorillonite are present in physical mixtures,

our models show that the proportions of these two end members vary systematically and can be discerned using PCA (Fig. 2); this variation in the spectra is greatest at 2.2 microns (an Al-OH vibration). Our results suggest that the presence and shape of the Al-OH and Fe/Mg-OH absorptions near 2.2 and 2.3 microns have the greatest influence over the position of samples in PC space. Understanding the specific types of phyllosilicates present on the martian surface is essential for interpreting the aqueous environments in which they formed. The PCA models of second-derivative NIR data from phyllosilicates presented here demonstrates that this method can correctly cluster phyllosilicates of similar compositions and abundances, and thus is a useful tool for elucidating past aqueous processes on Mars.

References: [1] Bibring J.-P. et al. (2006) *Science*, 312, 400-404. [2] Mustard J. F. et al. (2008) *Nature*, 454, 305-309. [3] Pelkey S. M. et al. (2007) *JGR*, 112, doi:10.1029/2006JE002831. [4] Ehlmann B. L. et al. (2009) *JGR*, 114, doi:10.1029/JE003339. [5] Robert P. et al. (1987) *Anal. Chem.*, 59 (17), 2187-2191. [6] Smith M. O. et al. (1985) *JGR*, 90, C797-C804. [7] Clark R. N. et al. (2007) USGS Digital Data Series 231. [8] Whitbeck M. R. (1981) *Appl. Spectrosc.*, 35, 93-95.

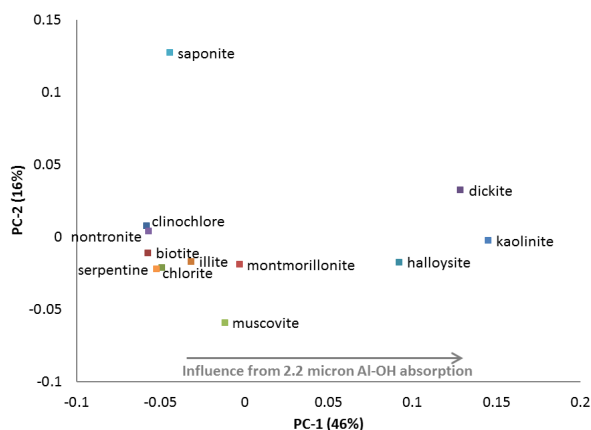


Figure 1. Scores plot for PC-1 (46%) and PC-2 (16%) of second-derivative NIR spectra of phyllosilicates in the USGS database. Percentages in parentheses represent the percent of variability in the data explained by each PC.

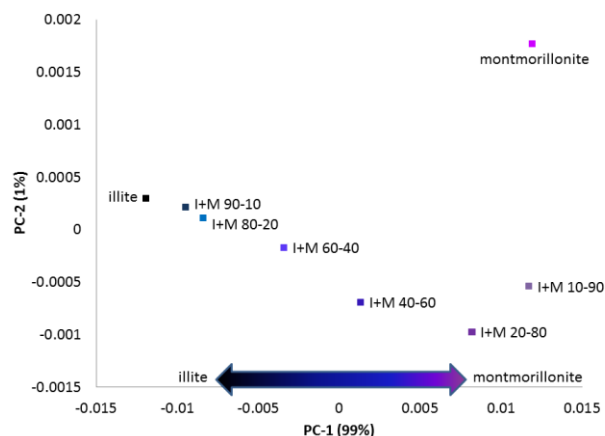


Figure 2. PCA model of second-derivative NIR spectra of illite-montmorillonite physical mixtures. Relative abundances (by weight) are noted. The PC-1 (99%) axis is controlled primarily by the Al-OH absorption near 2.2 microns.

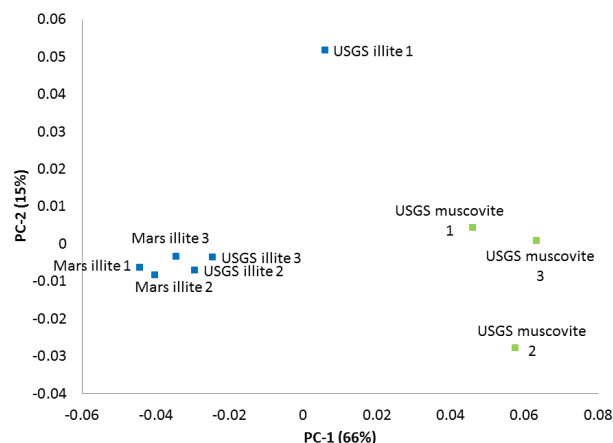


Figure 3. Scores plot for PC-1 (66%) and PC-2 (15%) of second-derivative NIR spectra of muscovite and illite in the USGS database and of illite/muscovite-rich regions in Nili Fossae. USGS muscovites 1, 2, and 3 correspond to samples Marshall, Tanzania, and HS, respectively. USGS illites 1, 2, and 3 correspond to samples 101, 105, and HS, respectively. Mars illites 1 and 2 are from [4] and Mars illite 3 is from [2]. Illites and muscovites are generally well clustered, with the martian data plotting close to the majority of terrestrial illite standards.